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► To cite this version:

Sébastien Brisard. Overview of FFT-based homogenization techniques from the Galerkin point of view. Conférence Internationale de Géotechnique, des Ouvrages et Structures (CIGOS 2015), ENS Cachan, May 2015, Cachan, France. hal-01194693

HAL Id: hal-01194693

<https://hal-enpc.archives-ouvertes.fr/hal-01194693>

Submitted on 7 Sep 2015

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Overview of FFT-based homogenization techniques from the Galerkin point of view

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Abstract

Most engineering materials are highly heterogeneous at various length-scales. As a consequence it is highly impractical to build a model of a structure which would encompass all heterogeneities. Fortunately, when length-scales are separated, homogenization theory can help account in a simplified way for the heterogeneity of the material making-up the structure.

A typical multiscale simulation based on homogenization theory is a two-step process. In a first step, the so-called corrector problem formulated over a representative volume element (with adequate boundary conditions) is solved. The macroscopic (homogenized) properties of the heterogeneous material are then retrieved from the solution to this corrector problem. In a second step, a full model of the structure is built, in which the heterogeneous materials are given their homogenized properties as per the previous step.

The present paper focuses on the numerical solution to the corrector problem (step 1). For complex microstructures with convoluted interfaces, it might become very difficult to build a conforming mesh, which rules out standard finite element simulations. In such complex situations, numerical methods formulated over regular grids might be preferable.

In the method initially proposed by [Moulinec and Suquet \(1994, 1998\)](#), the corrector problem is first reformulated as an integral equation (also known as the Lippmann–Schwinger equation), which is then discretized over a regular grid. The popularity of this method comes from the use of the fast Fourier transform (FFT) to compute efficiently the convolution product appearing in the Lippmann–Schwinger equation with periodic boundary conditions. Since the publication of the original paper, many variants of the so-called basic scheme have been introduced.

This method was recently revisited ([Brisard and Dormieux, 2012](#)) and a new formulation as a Galerkin discretization of the Lippmann–Schwinger equation was proposed. This approach leads to a unified framework for all variants of the basic scheme. In particular, the concept of discrete Green operator which stem from asymptotically consistent Galerkin discretizations of the Lippmann–Schwinger equation was introduced.

This paper briefly reviews FFT-based homogenization methods, with a focus on the Galerkin point of view.

Keywords: homogenization, elasticity, FFT

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1. Periodic homogenization and the corrector problem

This section briefly recalls the fundamentals of homogenization theory. The reader is referred to standard textbooks for more details (see e.g. [Milton, 2002](#); [Dormieux et al., 2006](#); [Auriault et al., 2009](#)). The mathematical theory of homogenization is also well established (see e.g. [Bensoussan et al., 1978](#); [Cioranescu and Donato, 1999](#); [Jikov et al., 1994](#)).

In the present paper, we consider a linearly elastic structure \mathcal{S} subjected to body forces $\mathbf{b}(\mathbf{x})$ ($\mathbf{x} \in \mathcal{S}$). The elastic equilibrium of this body is defined through the following partial differential equation over \mathcal{S}

$$\nabla \cdot (\mathbf{C} : \nabla^s \mathbf{u}) + \mathbf{b} = \mathbf{0}, \quad (1)$$

complemented with the following boundary conditions on $\partial\mathcal{S}$

$$\mathbf{u}|_{\partial\mathcal{S}} = \mathbf{0} \quad (2)$$

where \mathbf{u} (resp. $\boldsymbol{\varepsilon}$, $\boldsymbol{\sigma}$, \mathbf{C}) denotes the local displacement (resp. strain, stress and stiffness). It should be noted that Eq. (2) may be replaced with any other boundary conditions (provided that the resulting problem is well-posed).

Because of the heterogeneity of the constitutive material (\mathbf{C} may vary over the structure \mathcal{S}), solving Eqs. (1) and (2) can become a daunting task. Fortunately, in many engineering use cases, separation of scales prevails. In other words, the typical size ℓ of the heterogeneities is several orders of magnitude smaller than the typical size L of the structure \mathcal{S} : $\ell \ll L$.

In such situations, homogenization theory can be invoked, and Eq. (1) may be replaced with the following problem of elastic equilibrium of a *homogeneous* body

$$\nabla \cdot (\mathbf{C}^{\text{eff}} : \nabla^s \mathbf{u}) + \mathbf{b} = \mathbf{0}, \quad (3)$$

complemented with the same boundary conditions (2). In Eq. (3), the *constant* tensor \mathbf{C}^{eff} denotes the homogenized stiffness, to be defined below.

Although the results presented below can be extended to *random homogenization*, it is convenient to assume that the microstructure is *periodic*. In other words, the constitutive material of the structure \mathcal{S} is made of the repetition of a prismatic unit cell \mathcal{U} . For the sake of simplicity, the present paper will be restricted to cubic unit cells, $\mathcal{U} = (0, \ell)^d$, where ℓ is the size of the unit-cell and d is the spatial dimension. The homogenized stiffness is then defined as follows. Let \mathbf{u}^{per} be the unique (up to an additive constant) periodic solution to the *corrector problem* (formulated over \mathcal{U})

$$\nabla \cdot (\mathbf{C} : (\mathbf{E} + \nabla^s \mathbf{u}^{\text{per}})) = \mathbf{0}, \quad (4)$$

from \mathbf{u}^{per} , we can define the total strain $\boldsymbol{\varepsilon}$ and stress $\boldsymbol{\sigma}$

$$\boldsymbol{\varepsilon} = \mathbf{E} + \nabla^s \mathbf{u}^{\text{per}}, \quad \boldsymbol{\sigma} = \mathbf{C} : \boldsymbol{\varepsilon}, \quad (5)$$

and it is readily verified that $\bar{\boldsymbol{\varepsilon}} = \mathbf{E}$, which is called the macroscopic strain¹.

¹In the present paper, overlined quantities denote volume averages over the unit cell

$$\bar{\boldsymbol{\varepsilon}} = \frac{1}{|\mathcal{U}|} \int_{\mathbf{x} \in \mathcal{U}} \boldsymbol{\varepsilon}(\mathbf{x}) dV_{\mathbf{x}}.$$

Because of the linearity of Eq. (4), \mathbf{u}^{per} depends linearly on the sole loading parameter, namely the macroscopic strain \mathbf{E} . This is also true of the macroscopic stress $\bar{\boldsymbol{\sigma}}$, and the homogenized stiffness \mathbf{C}^{eff} is defined as the fourth-order tensor which maps the macroscopic strain to the macroscopic stress

$$\bar{\boldsymbol{\sigma}} = \overline{\mathbf{C} : \boldsymbol{\varepsilon}} := \mathbf{C}^{\text{eff}} : \mathbf{E} = \mathbf{C}^{\text{eff}} : \bar{\boldsymbol{\varepsilon}}. \quad (6)$$

Eq. (6) above shows how the homogenized stiffness can be retrieved from the solution to the corrector problem defined by Eq. (4). This homogenized stiffness can then be substituted in Eq. (3) to compute the mechanical fields in the whole structure \mathcal{S} .

Solving Eq. (3) is fairly standard structural analysis, and the remainder of this paper is devoted to solving Eq. (4) numerically. At this point, it should be recalled that this problem is formulated on the unit cell \mathcal{U} , which is assumed to be much smaller than the structure \mathcal{S} . However, \mathbf{C} may vary within \mathcal{U} , and approximating the solution to Eq. (4) through e.g. finite elements may remain difficult (see for example the microstructure pictured in Fig. 1, left). In such situations, the numerical technique presented below might be attractive.

The remainder of this paper is organized as follows. In Sec. 2, it is shown that Eq. (4) can be transformed into an integral equation known as the Lippmann–Schwinger equation. Then, in Sec. 3, this equation is discretized through a Galerkin approach. Sec. 4 shows that the resulting linear system can be solved efficiently in Fourier space. Finally, some examples are provided in Sec. 5.

2. The Lippmann–Schwinger equation

In the present section, Eq. (4) is transformed into an integral equation. This requires the introduction of the Green operator for strains, which is defined as follows. We consider the following auxiliary problem of the equilibrium over the unit cell \mathcal{U} of a *prestressed*, *homogeneous*, linearly elastic, reference material with stiffness \mathbf{C}_0

$$\nabla \cdot (\mathbf{C}_0 : \nabla^s \mathbf{u}^{\text{per}} + \boldsymbol{\varpi}) = \mathbf{0}, \quad (7)$$

where $\boldsymbol{\varpi}$ denotes the prestress (symmetric, second-order tensor field) and \mathbf{u}^{per} is the unknown periodic displacement induced by $\boldsymbol{\varpi}$. It can readily be shown that the derived strain field results from the convolution of $\boldsymbol{\varpi}$ with a kernel $\boldsymbol{\Gamma}_0$

$$\nabla_{\mathbf{x}}^s \mathbf{u}^{\text{per}} = - \int_{\mathbf{y} \in \mathcal{U}} \boldsymbol{\Gamma}_0(\mathbf{x} - \mathbf{y}) : \boldsymbol{\varpi}(\mathbf{y}) dV_{\mathbf{y}} = -(\boldsymbol{\Gamma}_0 * \boldsymbol{\varpi})(\mathbf{x}), \quad (8)$$

where $\boldsymbol{\Gamma}_0$ is the Green operator for strains. Taking advantage of the periodic boundary conditions, both $\boldsymbol{\varpi}$ and $\boldsymbol{\Gamma}_0 * \boldsymbol{\varpi}$ can be developed in Fourier series

$$\boldsymbol{\varpi}(\mathbf{x}) = \sum_{b \in \mathbb{Z}^d} \hat{\boldsymbol{\varpi}}(b) \varphi_b(\mathbf{x}) \quad (9)$$

$$(\boldsymbol{\Gamma}_0 * \boldsymbol{\varpi})(\mathbf{x}) = \sum_{b \in \mathbb{Z}^d} \hat{\boldsymbol{\Gamma}}_0(b) : \hat{\boldsymbol{\varpi}}(b) \varphi_b(\mathbf{x}) \quad (10)$$

where the basis functions φ_b and Fourier modes $\hat{\boldsymbol{\varpi}}(b)$ are given by

$$\varphi_b(\mathbf{x}) = \exp \frac{2i\pi}{\ell} (b_1 x_1 + \cdots b_d x_d) \quad (11)$$

$$\hat{\boldsymbol{\varpi}}(b) = \frac{1}{|\mathcal{U}|} \int_{\mathbf{x} \in \mathcal{U}} \boldsymbol{\varpi}(\mathbf{x}) \varphi_{-b}(\mathbf{x}) dV_{\mathbf{x}} \quad (12)$$

For isotropic reference materials, closed-form expressions of the Fourier modes $\hat{\Gamma}_0(b)$ of the Green operator for strains are known (see [Appendix A](#)).

We are now ready to go back to the corrector problem. Introducing an arbitrary homogeneous reference material \mathbf{C}_0 and the *polarization* $\boldsymbol{\tau}$ defined by Eq. (13b) below, Eq. (4) is equivalent to finding a \mathcal{U} -periodic displacement field \mathbf{u}^{per} such that

$$\nabla \cdot (\mathbf{C}_0 : \nabla^s \mathbf{u}^{\text{per}} + \mathbf{C}_0 : \mathbf{E} + \boldsymbol{\tau}) = \mathbf{0}, \quad (13a)$$

$$\boldsymbol{\tau} = (\mathbf{C} - \mathbf{C}_0) : (\mathbf{E} + \nabla^s \mathbf{u}^{\text{per}}). \quad (13b)$$

From the definition of the Green operator for strains, it is readily seen that Eq. (13a) leads to

$$\nabla^s \mathbf{u}^{\text{per}} = -\Gamma_0 * \boldsymbol{\tau}. \quad (14)$$

Eliminating $\nabla^s \mathbf{u}^{\text{per}}$ with the help of Eq. (13b), we finally get the following integral equation, where the main unknown is the polarization $\boldsymbol{\tau}$

$$(\mathbf{C} - \mathbf{C}_0)^{-1} : \boldsymbol{\tau} + \Gamma_0 * \boldsymbol{\tau} = \mathbf{E}, \quad (15)$$

which is known as the Lippmann–Schwinger equation ([Korringa, 1973](#); [Zeller and Dederichs, 1973](#); [Kröner, 1974](#); [Nemat-Nasser et al., 1982](#)). Sec. 3 below addresses the numerical approximation of the solution to this equation.

3. Galerkin discretization of the Lippmann–Schwinger equation

The Lippmann–Schwinger equation was first discretized on a cartesian grid by [Moulinec and Suquet \(1994, 1998\)](#), using point collocation and truncation of Fourier series. In this seminal work, the authors noticed that in Eq. (15), each term can be computed efficiently: indeed, the first term is local in the real space (it does not couple the polarizations of two different cells), while the second term is local in Fourier space [it does not couple the Fourier modes of the polarization, see Eq. (10)]. Accordingly, [Moulinec and Suquet](#) proposed an iterative scheme which takes full advantage of the particular structure of Eq. (15): each iteration takes place alternatingly in the real and the Fourier spaces. The efficiency of the resulting scheme comes from the fact that discrete Fourier transforms are evaluated by means of the Fast Fourier Transform algorithm.

Since it was first introduced, many improvements of this scheme have been proposed (see e.g. [Eyre and Milton, 1999](#); [Michel et al., 2001](#); [Brisard and Dormieux, 2010](#); [Monchiet and Bonnet, 2012](#), among others). It has been applied in various practical situations, including complex, non-linear behaviors ([Michel et al., 2001](#); [Šmilauer and Bažant, 2010](#); [Lebensohn et al., 2011, 2012](#); [Monchiet and Bonnet, 2013](#)).

The mathematical analysis of such schemes was initiated by [Brisard and Dormieux \(2012\)](#), who reformulated them as asymptotically consistent Galerkin approximations of the variational form of the Lippmann–Schwinger equation. This led to a proof of convergence as the cell-size goes to zero, whereas all previous studies were dedicated to the convergence of the iterative scheme itself (at constant cell-size). It should be noted that an alternative Galerkin approach (using trigonometric collocation) was also proposed by [Vondřejc et al. \(2014\)](#). Error estimates were also recently obtained ([Schneider, 2014](#); [Brisard and Legoll, 2014](#)).

The Galerkin approximation of the Lippmann–Schwinger equation by cell-wise constant polarization fields is based on the variational form of Eq. (15)

$$\text{find } \boldsymbol{\tau} \in \mathbb{V} \text{ such that, for all } \boldsymbol{\varpi} \in \mathbb{V} : \quad a(\boldsymbol{\tau}, \boldsymbol{\varpi}) = \mathbf{E} : \overline{\boldsymbol{\varpi}}, \quad (16)$$

where the space of polarizations \mathbb{V} is defined in (Brisard and Dormieux, 2012) and the bilinear form a reads

$$a(\boldsymbol{\tau}, \boldsymbol{\varpi}) = \overline{\boldsymbol{\varpi} : (\mathbf{C} - \mathbf{C}_0)^{-1} : \boldsymbol{\tau}} + \overline{\boldsymbol{\varpi} : (\boldsymbol{\Gamma}_0 * \boldsymbol{\tau})}. \quad (17)$$

A Galerkin discretization of Eq. (15) is then obtained by solving Eq. (17) on a finite dimension subspace of \mathbb{V} . In the present case, we consider a tessellation of the unit cell \mathcal{U} by a cartesian grid. Let h denote the grid spacing, so that the number of cells in each direction is $N = \ell/h$ (the total number of cells is N^d). Cells are indexed by greek tuples $\beta = (\beta_1, \dots, \beta_d) \in \{0, \dots, N-1\}^d$, such that cell β is

$$\mathcal{C}_\beta^h = (\beta_1 h, (\beta_1 + 1)h) \times \dots \times (\beta_d h, (\beta_d + 1)h) \quad (18)$$

We then consider as discretization space $\mathbb{V}^h \subset \mathbb{V}$ the space of cell-wise constant polarization fields; $\boldsymbol{\tau}_\beta^h$ denotes the constant value of $\boldsymbol{\tau}^h \in \mathbb{V}^h$ over the cell \mathcal{C}_β^h , and $\hat{\boldsymbol{\tau}}_b^h$ their discrete Fourier transform

$$\hat{\boldsymbol{\tau}}_b^h = \sum_{b_1=0}^{N-1} \dots \sum_{b_d=0}^{N-1} \exp\left(-\frac{2i\pi}{N}(\beta_1 b_1 + \dots + \beta_d b_d)\right) \boldsymbol{\tau}_\beta^h, \quad (19)$$

which can be computed efficiently by means of the Fast Fourier Transform.

The Galerkin approximation of the solution to problem (16) is then defined by the following variational problem

$$\text{find } \boldsymbol{\tau}^h \in \mathbb{V}^h \text{ such that, for all } \boldsymbol{\varpi}^h \in \mathbb{V}^h : \quad a(\boldsymbol{\tau}^h, \boldsymbol{\varpi}^h) = \mathbf{E} : \overline{\boldsymbol{\varpi}^h}. \quad (20)$$

Since \mathbb{V}^h is a finite-dimensional subspace of \mathbb{V} , the above equation reduces to a standard linear system which is identified from the evaluation of $a(\boldsymbol{\tau}^h, \boldsymbol{\varpi}^h)$ for all $\boldsymbol{\tau}^h, \boldsymbol{\varpi}^h \in \mathbb{V}^h$. It was shown that (Brisard and Legoll, 2014; Brisard and Dormieux, 2010) this system reads

$$\sum_{\beta_1=0}^{N-1} \dots \sum_{\beta_d=0}^{N-1} (\mathbf{C}_\beta^h - \mathbf{C}_0)^{-1} : \boldsymbol{\tau}_\beta^h + \sum_{b_1=0}^{N-1} \dots \sum_{b_d=0}^{N-1} \text{DFT}_\beta^{-1} \left[\hat{\boldsymbol{\Gamma}}_{0,b}^{h,c} : \hat{\boldsymbol{\tau}}_b^h \right] = \mathbf{E}, \quad (21)$$

for all $\beta \in \{0, \dots, N\}^d$. In Eq. (21), \mathbf{C}_β^h denotes the equivalent stiffness of cell β and $\hat{\boldsymbol{\Gamma}}_{0,b}^{h,c}$ is the so-called consistent, discrete Green operator (Brisard and Dormieux, 2012). Both are defined more precisely in Appendix B [see Eqs. (B.1) and (B.2)].

To close this section, it should be noted that the present, variational approach can lead to rigorous bounds on the homogenized stiffness as was illustrated by Brisard and Dormieux (2010). This results from the application of the principle of Hashin and Shtrikman (1962).

4. Implementation of the method

One of the assets of the method is its ease of implementation: a basic, non-optimized version would amount to few tens lines of code only.

Eq. (21) is solved by means of iterative linear solvers, which require an efficient implementation of the matrix-vector product Barrett et al. (1994). Of course, a matrix-free approach is adopted. This means that the matrix of the system (21) is neither stored, nor even computed. Rather, the matrix-vector product is computed at each iteration by means of Eq. (21).

This equation clearly shows that the linear operator of the system to be solved is the sum of two terms: the first term is block-diagonal, while the second term is block-circulant. Matrix-vector products are therefore evaluated as the sum of two terms: the first term is computed in the real space, while the second term is computed in the Fourier space. Therefore, the cost of one matrix-vector product is dominated by the cost of two discrete Fourier transforms (one forward, one inverse) per component of $\boldsymbol{\tau}^h$.

To close this section, it should be noted that in practice, evaluating the consistent discrete Green operator $\hat{\mathbf{I}}_{0,b}^{h,c}$ is prohibitively costly. It is also unnecessary, since it is acceptable to replace it with an asymptotically consistent approximation, by e.g. truncation (Moulinec and Suquet, 1994, 1998), filtering (Brisard and Dormieux, 2012), finite differences (Wilot et al., 2014; Willot, 2015) or finite elements (Yvonnet, 2012) – see also (Brisard and Legoll, 2014) for a brief review of the merits of each approximation.

5. Example of application

The application presented in this section illustrates the ability of the method to capture the finest details of the mechanical fields which develop in complex microstructures. Computations were carried out with a home-made code. Fast Fourier transforms were computed by means of the FFTW² library, while the PETSc³ toolkit provided scalable iterative linear solvers.

The microstructure depicted on Fig. 1 (left) is a dense assembly of 10 000 oblate inclusions ($a/c = 8$). The total volume fraction of inclusions is 60 %. The macroscopic strain is purely deviatoric, $\mathbf{E} = \mathbf{e}_1 \otimes \mathbf{e}_2 + \mathbf{e}_2 \otimes \mathbf{e}_1$ and the elastic properties of the matrix (m) and inclusions (i) were chosen as follows

Matrix $\mu_m = 1, \nu_m = 0.3,$

Inclusions $\mu_i = 100, \nu_i = 0.2.$

The Lippmann–Schwinger equation (15) was discretized on a 1024^3 grid ($6.44 \cdot 10^9$ unknowns), and the simulation was run on 16 cores of an Intel Xeon E5-2643 (3.30 GHz, 762 Go) for about 24 h.

Fig. 1 (right) shows a section through the 3D map of the (1, 2) component of the polarization field $\boldsymbol{\tau}$. Due to the closeness of the inclusions and the high elastic contrast between inclusions and matrix, the mechanical fields exhibit high fluctuations, which are well captured by the method.

6. Conclusion

This paper provides a brief overview of FFT-based numerical homogenization techniques. It shows that adopting a Galerkin point of view provides a sound ground for the mathematical

²<http://www.fftw.org/> (last retrieved

³<http://www.mcs.anl.gov/petsc/>

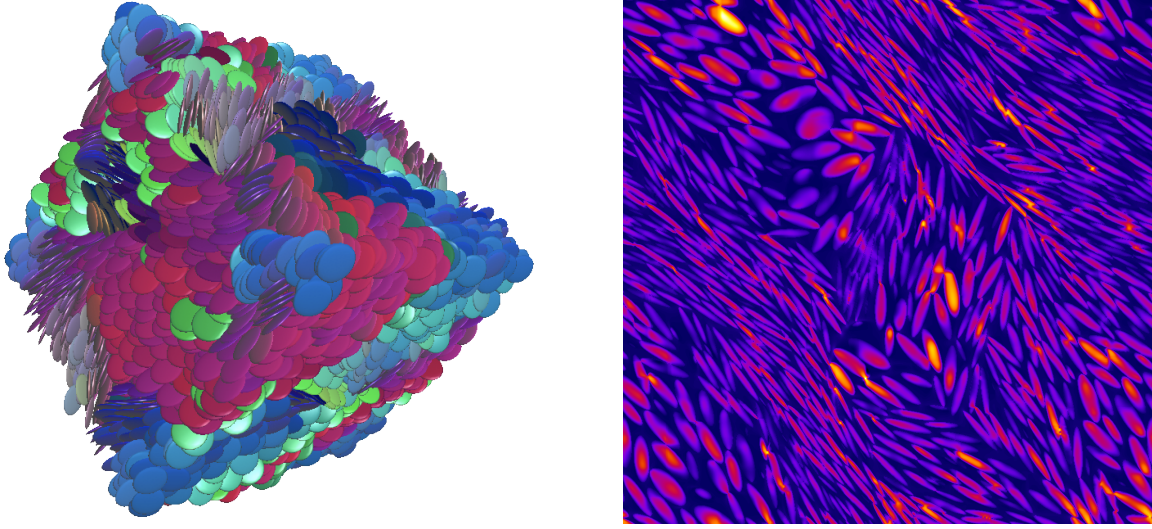


Figure. 1. The microstructure to be homogenized (left, reproduced from [Brisard and Levitz, 2013](#)), and a 2D cut through the 3D map of τ_{12} (right), for a macroscopic strain $\mathbf{E} = \mathbf{e}_1 \otimes \mathbf{e}_2 + \mathbf{e}_2 \otimes \mathbf{e}_1$. On 1024^3 grids, the method reveals fine details of the mechanical fields.

analysis of such schemes, as well as a unified framework for all the variants of the basic scheme.

Appendix A. The Green operator for strains

Closed-form expressions of the Fourier modes of the Green operator for strains can readily be derived (see e.g. [Suquet, 1990](#); [Nemat-Nasser et al., 1993](#)) when the reference material \mathbf{C}_0 is isotropic

$$\hat{\Gamma}_0(b) = \frac{1}{\mu_0} \text{sym}(\mathbf{n} \otimes \boldsymbol{\delta} \otimes \mathbf{n}) - \frac{1}{2\mu_0(1 - \nu_0)} \mathbf{n} \otimes \mathbf{n} \otimes \mathbf{n} \otimes \mathbf{n}, \quad (\text{A.1})$$

where μ_0 (resp. ν_0) is the shear modulus (resp. Poisson ratio) of the reference material, $\boldsymbol{\delta}$ is the second-order identity tensor, sym denotes symmetrization about the first and last two indices and

$$\mathbf{n} = (b_1^2 + \dots + b_d^2)^{-1/2} (b_1 \mathbf{e}_1 + \dots + b_d \mathbf{e}_d). \quad (\text{A.2})$$

Appendix B. Consistent discretization of the Lippmann–Schwinger equation

As shown in ([Brisard and Dormieux, 2010](#)), the equivalent stiffness of cell β is given by

$$\mathbf{C}_\beta^h = \mathbf{C}_0 + \left(h^{-d} \int_{\mathbf{x} \in \mathcal{C}_\beta^h} (\mathbf{C}(\mathbf{x}) - \mathbf{C}_0)^{-1} dV_{\mathbf{x}} \right)^{-1}. \quad (\text{B.1})$$

The above formula allows for *heterogeneous* cells. The consistent discrete Green operator allows for the exact calculation of $\overline{\boldsymbol{\varpi}^h} : (\boldsymbol{\Gamma}_0 * \boldsymbol{\tau}^h)$ for any $\boldsymbol{\tau}^h, \boldsymbol{\varpi}^h \in \mathbb{V}^h$. It is given by the following (slowly-converging) d -dimensional series ([Brisard and Dormieux, 2012](#))

$$\hat{\Gamma}_{0,b}^h = \sum_{n \in \mathbb{Z}^d} (F(b/N + n))^2 \hat{\Gamma}_0(b + nN) \quad \text{with} \quad F(u) = \prod_{i=1}^d \frac{\sin \pi u_i}{\pi u_i}. \quad (\text{B.2})$$

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